Russian Journal of General Chemistry 2005 vol.75 N6, pages 856-859

Structure and intramolecular lability of N-(Thio)phosphoryl(thio)amides: XIII. Structure of N-phenyl-N′-(diisopropoxythiophosphoryl)thiourea

Karataeva F., Yul'metov A., Zabirov N., Aganov A., Klochkov V.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

The structure and intramolecular transformations of N-phenyl--′-(diisopropoxythiophosphoryl)thiourea in (CD3) 2CO solution were studied by 1H, 13C, and 31P NMR spectroscopy. Combined analysis of NMR data and model calculations gave evidence in favor of high conformational and tautomeric flexibility of the thioureas in solution. The Z,E conformation of the amide form with the two N-H bonds cis and trans to the C=S bond was found to be preferred. © 2005 Pleiades Publishing, Inc.

http://dx.doi.org/10.1007/s11176-005-0333-8